

Electrical Conductivity of Fluid Oxygen at High Pressures

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Electrical conductivities of fluid oxygen were measured between 30 and 80 GPa at a few 1000 K. These conditions were achieved with a reverberating shock wave technique. The measured conductivities were several orders of magnitude lower than measured previously on the single shock Hugoniot because of lower temperatures achieved under shock reverberation. Extrapolation of these data suggests that the minimum metallic conductivity of a metal will be reached near 100 GPa.

[*experimental, liquid, oxygen, electrical conductivity, shock waves*]

1. Introduction

The study of the properties of simple diatomic molecular fluids at high pressure and density is a subject of increased interest in light of the recent experimental results on liquid hydrogen. Measurements of the electrical conductivity indicate that hydrogen reaches the minimum conductivity of a metal at 140 GPa and 9-fold compression [1,2]. The mass density at metallization and the measured electrical conductivity are consistent with the Goldhammer-Herzfeld criterion [3] and the Mott prediction for the minimum conductivity of a metal [4]. Although the hydrogen results are described well at the macroscopic level by such simple and general principles, the details of the transition at the microscopic level are not yet known. In order to advance our understanding of the fundamental electronic transport properties of warm fluids under such extreme conditions of pressure and density we looked at another simple molecular liquid – oxygen, which at ambient conditions is a wide gap insulator ($E_g=12$ eV).

2. Experiments

We measured the electrical resistivity of oxygen compressed by reverberating shocks starting from a liquid sample of density $\rho_0=1.2$ g/cm³ at $T_0=77$ K and $P_0=0.1$ MPa. The details of the technique, target construction and electrical circuitry are very similar to those of Ref. [1]. The high pressure and density conditions in the sample were maintained at constant level for durations of at least 100ns which allowed the system to equilibrate and the measurement to be taken. The target design was optimized to achieve highly homogeneous samples, to essentially eliminate thermal and pressure gradients and to maximize the accuracy of the measurement. In order to ensure that the triggering process did not interfere with the conductivity measurement, we mounted the pins that control the data acquisition system in the back of the target, such that the actual trigger occurred after the experiment was over. This is made possible by the long writing time of the fast digital recording system.

3. Discussion

The measured conductivity of fluid oxygen ranges from 10^{-4} (Ωcm)⁻¹ up to 50 (Ωcm)⁻¹ between 30 GPa and 80 GPa, respectively. These conductivity values are up to five orders of magnitude smaller than the conductivities observed along the principal Hugoniot at the same pressures [5]. Such a big difference

between the conductivities can be explained by the fact that the high-pressure states achieved in the shock reverberation technique are at significantly lower temperatures than on the Hugoniot. It is inferred, therefore, that the resistivity measured along the Hugoniot is mainly due to the high degree of thermal excitation of the carriers over the mobility gap. The maximum electrical conductivity measured using the shock reverberation technique is almost two orders of magnitude lower than the minimum conductivity of a metal. In order to understand how the energy gap closes with pressure one has to take into consideration several factors such as temperature, density and molecular dissociation fraction. The Mott criterion predicts that the Metal/Insulator transition occurs when $n_c^{1/3} a_B \sim 0.25$, where n_c is the critical density of centers providing conduction electrons and a_B is the radius of the maximum in the charge density of the outermost valence orbital of the atoms (or molecules). We calculated the distance between neighboring centers ($n^{-1/3}$) from the experimental density values and estimated a_B for the atomic and molecular oxygen species ($a_B^O=0.88$ a.u. and $a_B^{O_2}=1.2$ a.u.) using two quantum chemistry codes (GAMESS and SPARTAN). For the two extreme cases of entirely molecular and completely dissociated liquids we estimated the corresponding Mott scaling parameters and found that they differ by less than 10%. The pressure dependence of the electrical conductivity of liquid oxygen suggests that a minimum metallic conductivity of ~ 2000 (Ωcm)⁻¹ will be reached at a pressure around 100 GPa. At this pressure, the Mott scaling parameter corresponding to the two extreme cases of completely dissociated and fully molecular liquid was calculated to be 0.25 and 0.28 respectively. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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